

# Probable detection of $\text{H}_2\text{D}^+$ in the starless core Barnard 68

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## ABSTRACT

**Context.** The presence of  $\text{H}_2\text{D}^+$  in dense cloud cores underlies ion-molecule reactions that strongly enhance the deuterium fractionation of many molecular species.

**Aims.** We determine the  $\text{H}_2\text{D}^+$  abundance in one starless core, Barnard 68, that has a particularly well established physical, chemical, and dynamical structure.

**Methods.** We observed the ortho- $\text{H}_2\text{D}^+$  ground-state line  $1_{10}-1_{11}$ , the  $\text{N}_2\text{H}^+$   $J=4-3$  line, and the  $\text{H}^{13}\text{CO}^+$   $4-3$  line with the APEX telescope.

**Results.** We report the probable detection of the o- $\text{H}_2\text{D}^+$  line at an intensity  $T_{\text{mb}}=0.22 \pm 0.08$  K and exclusively thermal line width, and find only upper limits to the  $\text{N}_2\text{H}^+$   $4-3$  and  $\text{H}^{13}\text{CO}^+$   $4-3$  intensities.

**Conclusions.** Within the uncertainties in the chemical reaction rates and the collisional excitation rates, chemical model calculations and excitation simulations reproduce the observed intensities and that of o- $\text{H}_2\text{D}^+$  in particular.

**Key words.** ISM: abundances – ISM: individual objects: Barnard 68 – ISM: molecules – Submillimeter

## 1. Introduction

The densest and coldest cores of interstellar molecular clouds are receiving much attention as the possible precursors of star formation. Often referred to as starless or pre-protostellar cores, they are characterized chemically by a large depletion of molecules as they freeze out onto dust grains, and an associated increase in the relative abundance of deuterated isotopomers of numerous species (e.g., Kuiper et al. 1996; Ceccarelli et al. 1998; Loinard et al. 2002; Bacmann et al. 2003; Caselli et al. 2003; Stark et al. 2004). This increase is explained by the reaction  $\text{H}_3^+ + \text{HD} \rightleftharpoons \text{H}_2\text{D}^+ + \text{H}_2$ , which is favored in the forward direction at low temperatures, and subsequent ion-molecule reactions involving  $\text{H}_2\text{D}^+$ . Detection of  $\text{H}_2\text{D}^+$  in dense cloud cores directly tests this proposed mechanism. Through its spectral line shape it also probes the core's velocity field, in regions where all other molecular tracers are strongly depleted. First predicted by Dalgarno et al. (1973), the ground-

state transition of ortho- $\text{H}_2\text{D}^+$ ,  $1_{10}-1_{11}$ , lies in the submillimeter wavelength range near 372 GHz, in a region with poor atmospheric transmission. Under excellent observing conditions on Mauna Kea (Hawai'i),  $\text{H}_2\text{D}^+$  has been successfully detected toward astronomical sources, including the young stellar object NGC 1333 IRAS 4A (Stark et al. 1999), the starless core L1544 (Caselli et al. 2003), and the circumstellar disks of TW Hya and DM Tau (Ceccarelli et al. 2004; but also see Guilloteau et al. 2006). This Letter reports the probable detection of the  $\text{H}_2\text{D}^+$   $1_{10}-1_{11}$  line toward the well-studied starless core Barnard 68 conducted with the Atacama Pathfinder Experiment (APEX<sup>1</sup>) telescope on Chajnantor (Chile).

Barnard 68 (B68) is one of the most extensively studied starless cores. Using stellar extinction measurements, its density structure has been found to be well matched by a near-critical Bonnor-Ebert sphere (Alves et al. 2001). Bonnor-Ebert

<sup>1</sup> This publication is based on data acquired with the Atacama Pathfinder Experiment (APEX). APEX is a collaboration of the Max-Planck-Institut für Radioastronomie, the European Southern Observatory, and the Onsala Space Observatory.

spheres (Ebert 1957; Bonnor 1958) describe the equilibrium configuration of self-gravitating cloud cores just before the onset of collapse. Bergin et al. (2002) found strong depletion of  $\text{C}^{18}\text{O}$  in B68. Lada et al. (2003) analyzed the velocity field of B68, and found that the line widths in the center are close to thermal, leaving no room for significant turbulent motion. In the outskirts of the core, line centroid shifts suggest a non-radial pulsating motion.

With the successful commissioning of APEX, the 372 GHz ground-state transition of ortho- $\text{H}_2\text{D}^+$  has come within reach of regular observing, given the good local weather conditions. This Letter presents the probable detection of  $\text{H}_2\text{D}^+$  toward the center of this starless core obtained during the Science Verification of APEX (§2) and discusses the emission strength in the framework of a chemical model including depletion and deuteration (§3).

## 2. Observations and results

The APEX telescope observed the  $\text{H}_2\text{D}^+$   $1_{10}-1_{11}$  line at 372.421385 GHz on 2005 July 24 and 25 using the APEX-2a receiver and the FFTS backend with a bandwidth of 1 GHz and 16384 channels. This frequency setting also covers the  $\text{N}_2\text{H}^+$   $J=4-3$  line at 372.6725090 GHz. The telescope was pointed at the  $A_V$  peak measured by Alves et al. (2001) at  $\alpha_{2000} = 17^{\text{h}}22^{\text{m}}38^{\text{s}}.6$  and  $\delta_{2000} = -23^{\circ}49'46''.0$ . The observations were taken in position-switched mode, using an emission-free reference position. Pointing was checked on the nearby object RAFGL 1922. During the observations the source was at elevations of  $25^{\circ}$ – $40^{\circ}$ . A precipitable water vapor column of 0.47 mm resulted in DSB system temperatures of 150–250 K. On 2005 July 25, the  $\text{H}^{13}\text{CO}^+$   $J=4-3$  line at 346.998546 GHz was observed with a similar set up. After the observations, the velocity scale of the spectra was recalculated by the telescope staff to correct for a small ( $0.1 \text{ km s}^{-1}$ ) inaccuracy during data taking.

After careful inspection of the data, the individual 30 sec scans were averaged using the CLASS software package; a total integration time (on+off) of 36 min was obtained for the  $\text{H}_2\text{D}^+$  line (12.6 min for  $\text{H}^{13}\text{CO}^+$ ). A sinusoidal baseline with a period of  $\sim 350 \text{ km s}^{-1}$  was removed, followed by a first order baseline in the area surrounding the expected line. After smoothing the spectral resolution to  $0.098 \text{ km s}^{-1}$ , a rms noise level of  $0.059 \text{ K}$  on the  $T_A^*$  scale was found ( $0.058 \text{ K}$  for  $\text{H}^{13}\text{CO}^+$  in  $0.11 \text{ km s}^{-1}$  channels), adopting a forward efficiency of 0.97. The data were subsequently transformed to the main beam antenna temperature scale by division by 0.73, the recommended mean beam efficiency in the 345 GHz band (Güsten et al. 2006).

The  $\text{H}_2\text{D}^+$  line was detected at a signal-to-noise ratio of  $\sim 3$  (Fig. 1). Fitting a single Gaussian line to the spectrum yields  $T_{\text{mb}} = 0.222 \pm 0.082 \text{ K}$ ,  $V_{\text{LSR}} = 3.36 \pm 0.05 \text{ km s}^{-1}$ ,  $\Delta V = 0.33 \pm 0.1 \text{ km s}^{-1}$ , and an integrated line intensity of  $0.078 \pm 0.015 \text{ K km s}^{-1}$ . Although the line peak is detected at only  $2.7\sigma$ , the integrated intensity is detected at  $5.2\sigma$ , and we argue that the detection of  $\text{H}_2\text{D}^+$  in B68 is probable (only deeper integration can make the result more secure). Fig. 3 in the on-line material shows the  $\text{H}_2\text{D}^+$  spectrum over a

$200 \text{ km s}^{-1}$  range. Out of the 1018 channels in this part of the spectrum, only 4 exceed the  $3\sigma$  level (0.4%), as statistically expected. The significance of the detection is further supported by the close match to the source  $V_{\text{LSR}}$  of  $3.36$ – $3.37 \text{ km s}^{-1}$  and the purely thermal line width of  $0.33 \text{ km s}^{-1}$  ( $\text{H}_2\text{D}^+$  at  $10 \text{ K}$ ), as found by Lada et al. (2003) for  $\text{N}_2\text{H}^+$  and  $\text{C}^{18}\text{O}$ . All other peaks are much narrower (1–2 channels). Because  $\text{H}_2\text{D}^+$  retains a high abundance at the center of the core (see below), the apparent absence of turbulent motion in the  $\text{H}_2\text{D}^+$  line provides strong support for the conclusion of Lada et al. (2003) that B68 is exclusively thermally supported. This situation is very different from the velocity field in, e.g., L1544, which shows significant velocity gradients and wider  $\text{H}_2\text{D}^+$  lines (van der Tak et al. 2005). No detection was made of either the  $\text{N}_2\text{H}^+$   $4-3$  line to a  $2\sigma$  upper limit of  $0.16 \text{ K}$  or the  $\text{H}^{13}\text{CO}^+$   $4-3$  line to  $2\sigma$  of  $0.18 \text{ K}$ . An emission peak at the correct  $V_{\text{LSR}}$  for the  $\text{N}_2\text{H}^+$  transition and the expected thermal width of  $0.075 \text{ km s}^{-1}$  is likely noise.

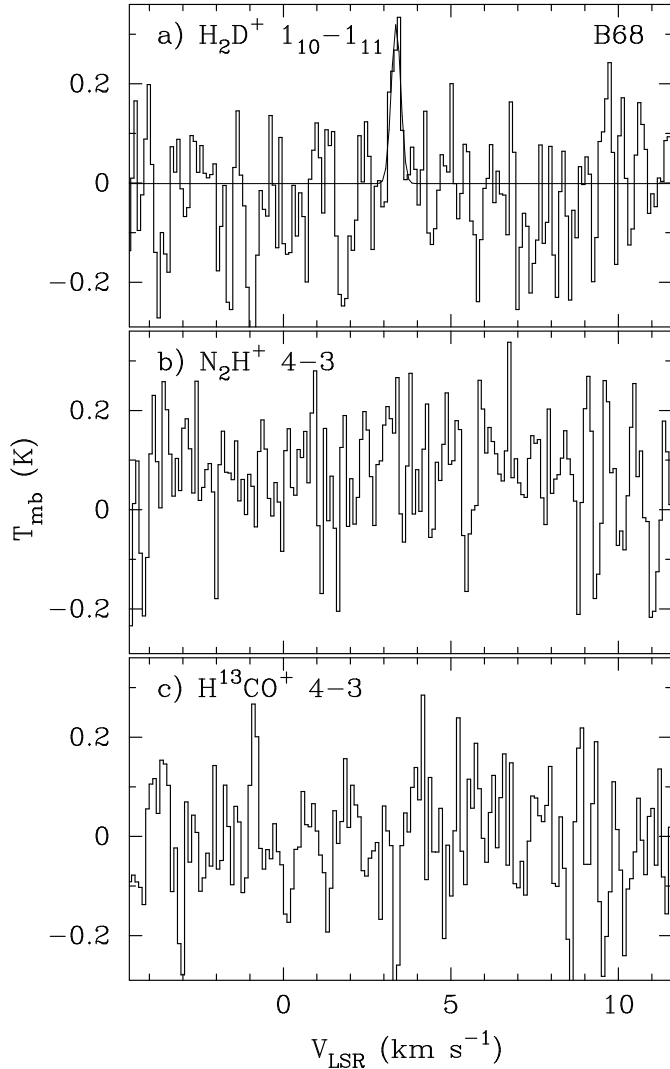
In the documents accompanying the data release, it was noted that lines tuned in the upper sideband of APEX-2a could be too strong by 40%. This effect has been shown to be present for  $^{12}\text{CO}$   $J=3-2$ , and is thought to be due to a resonance near the CO line frequency. It is therefore unlikely that our  $\text{H}_2\text{D}^+$  observations suffer from this effect, although no sideband-ratio measurements are available to confirm this.

## 3. Discussion

At the detected line strength of  $0.22 \pm 0.08 \text{ K}$ , the  $\text{H}_2\text{D}^+$  line is weaker than detections toward other starless cores such as L1544 ( $\sim 1 \text{ K}$ ). Two aspects distinguish B68 from L1544. First, B68's  $\text{H}_2$  column density is lower than that of L1544, at  $3.6 \times 10^{22} \text{ cm}^{-2}$  and  $(6-13) \times 10^{22} \text{ cm}^{-2}$  (Alves et al. 2001; Ward-Thompson et al. 2002, 1999). Secondly, B68's central density of  $2 \times 10^5 \text{ cm}^{-3}$  is lower by a factor of 6 than that of L1544. Given that the critical density of the ground-state transition of ortho- $\text{H}_2\text{D}^+$  is  $\sim 2 \times 10^6 \text{ cm}^{-3}$  (for our adopted collision rate; see below), a careful analysis is required to test whether the decreased line strength is due to (a combination of) sub-thermal excitation, lower total column density, or lower abundance of this key deuterated species.

From the strength of the  $\text{H}_2\text{D}^+$  line, assuming optically thin conditions, we derive a beam-averaged column density of  $N(\text{H}_2\text{D}^+) = (1.5 \pm 0.14) \times 10^{12} \text{ cm}^{-2}$  for an excitation temperature of  $10 \text{ K}$ . This corresponds to thermal equilibrium excitation at the kinetic temperature in B68. Given the critical density quoted above, it is highly likely that the excitation is subthermal, requiring a larger column density to reproduce the emission. For example, an excitation temperature of  $5 \text{ K}$  implies  $N(\text{H}_2\text{D}^+) = (1.0 \pm 0.3) \times 10^{13} \text{ cm}^{-2}$ . This column density corresponds to an average  $\text{H}_2\text{D}^+$  abundance with respect to  $\text{H}_2$  of  $(2.9 \pm 0.9) \times 10^{-10}$ .

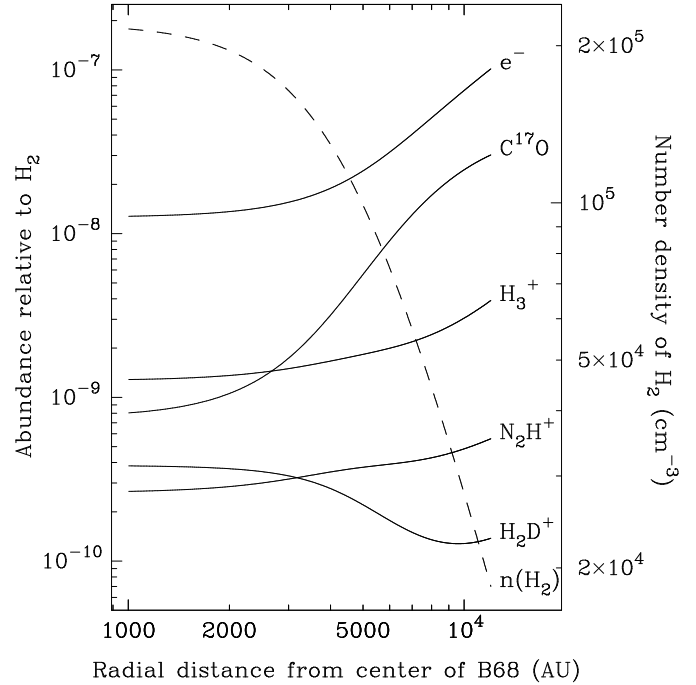
Further insight in the  $\text{H}_2\text{D}^+$  abundance can be obtained from modeling the chemistry in the B68 core followed by a statistical equilibrium calculation of the  $\text{H}_2\text{D}^+$  excitation and line radiative transfer. Following Vastel et al. (2006) we use the simple chemical model of Caselli et al. (2002), updated to include the multiply deuterated forms of  $\text{H}_3^+$  and the new val-



**Fig. 1.** (a) Detection spectrum of  $\text{H}_2\text{D}^+$   $1_{10-1_{11}}$  toward the center of B68 (histogram), with the best-fit Gaussian line profile superposed (thin line). The model of §3 yields an identical profile for the modified collisional excitation rates as discussed. (b) Non-detection of  $\text{N}_2\text{H}^+$   $4-3$  at the same position. (c) Non-detection of  $\text{H}^{13}\text{CO}^+$   $4-3$  at the same position.

ues of the binding energies of CO and  $\text{N}_2$  (Öberg et al. 2005). B68 is modeled as a spherical cloud with radius 12,000 AU and the density profile fitted to the Bonnor-Ebert solution by Tafalla et al. (2002, 2004). The temperature profile follows that of L1544 (Young et al. 2004), resulting in a temperature gradient from 13 K at the core edge to 9.8 K at its center.

The chemical model starts with fully undepleted abundances of CO,  $\text{N}_2$ , and O, and lets the species interact with and freeze-out on the dust grains which follow a MRN size distribution (Mathis et al. 1977) with a minimum grain size of  $0.005 \mu\text{m}$ . Assuming that the ion chemistry is fast compared to depletion, the molecular ions follow from the instantaneous neutral abundances. Following Vastel et al. (2006) a cosmic-ray ionization rate of  $1.3 \times 10^{-17} \text{ s}^{-1}$  and sticking coefficient to  $S = 1.0$  (Burke & Hollenbach 1983) are adopted. Finally, for  $\text{H}_2\text{D}^+$  an ortho-to-para ratio of 1.0 is adopted as expected



**Fig. 2.** Predicted abundances of several key species in the  $\text{H}_2\text{D}^+$  modeling (solid lines) and  $\text{H}_2$  number density (dashed line) as functions of radius in B68.

at low temperatures (Gerlich et al. 2002). We note that the results of these calculations may depend quite sensitively on the chemical reaction rates and their dependence on temperature (Emprechtinger et al. in preparation), including the  $\text{H}_2\text{D}^+$  destruction reaction with  $\text{H}_2$  (Schlemmer et al. 2005 and Asvany et al., in preparation).

Figure 2 shows the resulting abundance profiles of some relevant species. Typical  $\text{H}_2\text{D}^+$  abundances with respect to  $\text{H}_2$  at the center of B68 are predicted to be  $4 \times 10^{-10}$ . The corresponding  $\text{H}_2\text{D}^+$  column density is  $5.0 \times 10^{12} \text{ cm}^{-2}$ , close to the beam-averaged column density of  $1 \times 10^{13} \text{ cm}^{-2}$  found from the simple analysis above.

With these abundance profiles, the statistical equilibrium excitation is calculated using the code of Hogerheijde & van der Tak (2000). The velocity field is assumed to be static with only thermal broadening and no turbulent motion. We ignore the significant motion in the outer regions of the core reported by Lada et al. (2003), since our observations are taken to the core's center and the observed spectrum shows no indication of line broadening. The resulting spectrum is convolved in a  $17''$  FWHM beam appropriate for APEX at these wavelengths, yielding intensities on the  $T_{\text{mb}}$  scale; a distance of 100 pc is adopted for B68.

These calculations require reliable collisional rate coefficients, which are not available in the literature. We follow van der Tak et al. (2005) in adopting estimated rates, and investigate the effect of their inherent uncertainty. Using these rates, we find a  $\text{H}_2\text{D}^+$   $1_{10-1_{11}}$  intensity of 0.10 K, lower by a factor of 2 than observed. Increasing the collisional rates by a factor of three, entirely within the estimated uncertainty, increases the emergent intensity to 0.24 K. Varying the rates by factors of 10

up or down produces a range of intensities of 0.011–0.48 K. The opacity of the line is 0.13 and the excitation temperature ranges from 3 to 6 K, consistent with the simple assumptions made above.

We conclude that the observed intensity of  $\text{H}_2\text{D}^+$  is consistent with chemical model predictions, but that the uncertainty in the available collisional rate coefficients precludes a detailed comparison, especially for subthermal excitation. Determination of more reliable rates is clearly warranted. van der Tak et al. (2005) reach the same conclusion, including a preference for collision rates enhanced by factors 3–10; like these authors, we refrain from recommending adjusting the collision rates because of the uncertainties in the chemical modeling.

Using collisional rates from the Leiden data base (Schöier et al. 2005), our model calculations are compatible with the upper limits on  $\text{H}^{13}\text{CO}^+$  and  $\text{N}_2\text{H}^+$  4–3 reported here, as well the  $\text{N}_2\text{H}^+$  and  $\text{C}^{18}\text{O}$  1–0 detections of Bergin et al. (2002) and  $\text{N}_2\text{H}^+$  3–2 from Crapsi et al. (2005). Quantitatively, we find 19 mK for  $\text{H}^{13}\text{CO}^+$  4–3 (observed:  $< 0.15$  K,  $2\sigma$ );  $0.79$  K  $\text{km s}^{-1}$  for  $\text{C}^{18}\text{O}$  1–0 ( $0.85$  K  $\text{km s}^{-1}$ ). Our model overproduces the  $\text{N}_2\text{H}^+$  emission by about a factor of 2; we find  $0.38$  K for  $\text{N}_2\text{H}^+$  4–3 (observed  $< 0.16$  K,  $2\sigma$ ), and values of  $3.8$  K  $\text{km s}^{-1}$  for  $\text{N}_2\text{H}^+$  1–0 (observed,  $2.5$  K  $\text{km s}^{-1}$ ) and  $0.35$  K  $\text{km s}^{-1}$  for 3–2 (observed,  $0.17$  K  $\text{km s}^{-1}$ ).

We conclude that our detection of  $\text{H}_2\text{D}^+$  toward B68 is consistent with models for the deuterium chemistry in starless cores which also reproduces other observed lines. However, the lack of reliable collision rates precludes any stronger statements about the  $\text{H}_2\text{D}^+$  chemistry. Given the pivotal role of  $\text{H}_2\text{D}^+$  in deuterium chemistry and the well studied nature of B68, calculation of such rates is warranted, especially now that observations of  $\text{H}_2\text{D}^+$  ground-state transition are possible with APEX. In the future, ALMA observations of the resolved emission of  $\text{H}_2\text{D}^+$  and other species will provide further insight into the chemical state of B68, and only with reliable collision rates will quantitative analysis of these observations be possible.

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# Online Material

## List of Objects

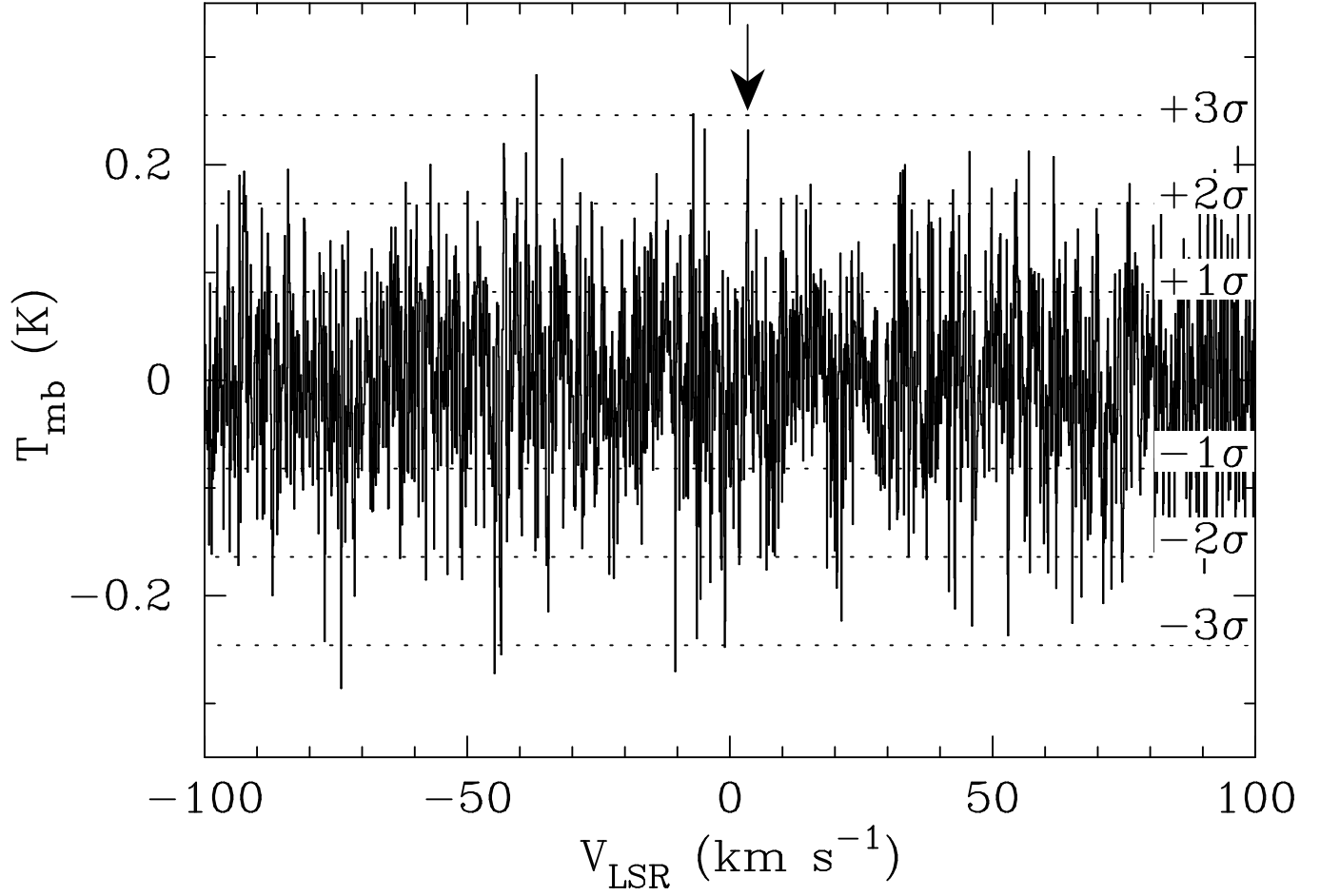
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‘L1544’ on page 1

‘TW Hya’ on page 1

‘DM Tau’ on page 1

‘Barnard 68’ on page 1



**Fig. 3.** Detection spectrum of  $\text{H}_2\text{D}^+$   $1_{10}-1_{11}$  toward the center of B68 over a baseline range of  $200 \text{ km s}^{-1}$ . Noise levels at  $\pm 1\sigma$ ,  $\pm 2\sigma$ , and  $\pm 3\sigma$  are indicated. The arrow indicates the  $V_{\text{LSR}}$  of B68 of  $3.36 \text{ km s}^{-1}$ .